Pentanedioic acid, hexafluoro-376-73-8 | DTXSID8059926

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 308 °C

Global applicability domain: Outside

Local applicability domain index: 2.09e-01

Confidence level: 6.11e-01

Nearest Neighbors from the Training Set

Image not found

Hexanedioic acid Measured: 338 Predicted: 330 Image not found

Pentanedioic acid Measured: 303 Predicted: 310 Image not found

Heptanedioic acid Measured: 342 Predicted: 332

Image not found

1-Perfluorobutanesulfonic acid

Measured: 211 Predicted: 212 Image not found

Octanedioic acid Measured: 346 Predicted: 332